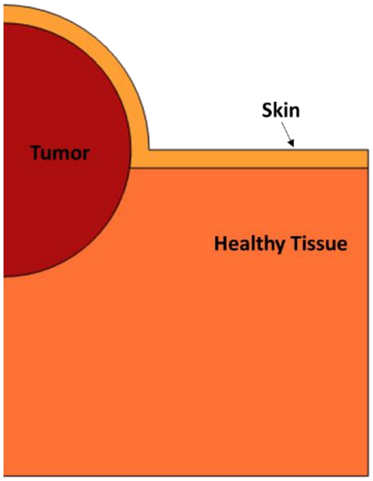
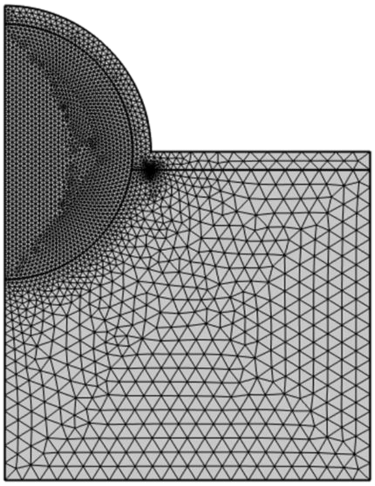
Supplemental Data 1 – Thermal Modeling





2D modeling of the tumor. For the modeling of the tumor, a 2D axisymmetric physical model for spherical tumors surrounded by an adjacent healthy tissue and skin from the above in a cylindrical form was assumed. The physical dimensions are set as 0.5mm of thickness and 10 mm in length for skin above the tumor, 7 mm as the diameter of the tumor and 8 mm of thickness and 10 mm of length for healthy tissue. It was assumed that the physical model's top surface is illuminated by a collimated Gaussian laser beam.

The Bioheat equation (**Eq.1**)(1) is defined as the follows: first, the left-hand term $\rho C_p \frac{\partial T}{\partial t}$ represent the rate of energy storage, where ρ is the tissue density [kg/m^3], C_p is the tissue specific heat [*J / (kg·K)*] and t is the time [*s*]. The first term on the right-hand side, $\nabla(k\nabla T)$, is the loss of thermal energy due to conduction, where T is the temperature and k is the tissue thermal conductivity [*W/ m·K*]. $\rho_b C_b \omega_b (T_b - T)$ is the approximate local loss of energy due to the blood flow in capillaries, where ρ_b is the blood density [kg/m^3], C_b is the blood specific heat [*J / (kg·K)*], ω_b is the blood perfusion rate [*1/s*] and T_b is the arterial blood temperatures [K]. Lastly, the terms Q_{met}, Q_{laser} represent the metabolic heat generation rate [W/m^3] and the external laser source

[W/m^3], respectively. The parameters used for the Bioheat transfer equation is listed in **Table S1**, and the thermal properties of the various tissues are listed in **Table S2**.

Eq. 1

$$\rho C_p \frac{\partial T}{\partial t} = \nabla(k\nabla T) + \ \rho_b C_b \omega_b (T_b - T) + Q_{met} + Q_{laser}$$

Eq. 2 was used to define the boundary between the tumor surface and the surrounding environment, where n is the unit vector normal to the surface, h is the heat transfer coefficient [Wm^{-2}K^{-1}], T_{ext} is the temperature boundary, and T is the ambient temperature environment at 20 ^{o}C. The term on the right side of this equation describes the heat losses due to convection.

Eq. 2

$$-\, n \cdot (-k\nabla T) = h \cdot (T_{ext} - T)$$

Next, the optical properties of the laser parameters, the carbon nanotubes and tissues are defined. The laser used was a continuous laser with an assumed Gaussian beam shape defined in cylindrical coordinate as follows:

Eq. 3

$$Q_{laser}(r,z) = \frac{-\partial I(r,z)}{\partial z} = \ \mu_a I_o (1 - R) \exp[-(\mu_a + \mu_s) z] \exp\left[-\frac{2r^2}{w(z)^2}\right]$$

where $\frac{-\partial I(r,z)}{\partial z}$ is the intensity attenuated through tissue depth in the - z-direction, I_o is the incident laser power density, $w(z) = \ w_o \sqrt{1 + \left(\frac{z}{z_r}\right)^2}$ is the beam radius that depends upon the position in the - z-direction, $z_R = \frac{\pi w_o^2}{\lambda}$ is the Rayleigh length with the parameter w_o define as the beam waist and λ is the wavelength of the laser. The parameter R is the spectral reflectivity at the air-tissue interface, defined as $R = \left(\frac{n_1 - n_2}{n_1 + n_2}\right)^2$ where n_1 and n_2 are defined as the refractive index of tissue and air, respectively. The laser source parameters used to calculate the laser properties are listed in **Table S3**.

The optical properties of carbon nanotubes within the tissue volume are defined as μ_a and μ_s . The parameter $\mu_a = \mu_{am} + \mu_{an}$ represents the absorption coefficient, where the terms μ_{am} and μ_{an} are the absorption coefficient for the mouse tissue and the absorption coefficient for the MWCNTs, respectively. The parameter $\mu_s = \mu_{sm} + \mu_{sn}$ represents the scattering coefficient, where the terms μ_{sm} and μ_{sn} are the scattering coefficient for the mouse tissue and for the MWCNTs, respectively. Thus, the scattering coefficient for the tissue is defined as $\mu_{sm} = (1 - g)u_s$. The quantities μ_{an} and μ_{sn} are calculated as follows:

Eq. 4

$$\mu_{an} = f_v \frac{3\, Q_a}{4\, r_{eff}}$$

Eq. 5

$$\mu_{sn} = f_v \frac{3\, Q_s}{4\, r_{eff}}$$

Where $r_{eff} = \left(\frac{3V}{4\pi}\right)^{1/3}$ is the effective radius of the CNTs, f_v is volume fraction and Q_s is the dimensionless scattering efficiency factor for a single CNT. The nanoparticle distribution within the tumor region is assumed intravenously injected, and as such 0.9% of the injected CNTs were assumed to accumulate at the tumor(2). Therefore, the volume fraction of nanoparticles, introduced and proposed by Dombrovsky *et al.*(3), will be used to link the amount of radiant energy penetration in the tissue. The list of optical properties of the different tissues are listed in **Table S4**.(4)

Table S1. Parameters used for the Bioheat transfer equation.

Parameters	**Values**	**Units**
Heat transfer coefficient *h*	10	[W/m^{2}K]
Reflectivity *R*	0.027	-
Temperature body	36.6	[ºC]
Ambient temperature	20	[ºC]
Volume fraction f_v	6.63 x 10^{-7}	-

Table S2. Thermal properties of the tumor, the healthy tissue and skin*(4-7)*.

Parameters	**Skin (animal)**	**Fat (animal)**	**Thyroid Gland (human)**	**Bakground tissues (human)**	**Thyroid tumor (human)**	**Blood**	**Units**
Density ρ	1180	1000	1050	1090	1000	1060	[kg/m^3]
Specific heat C	2291	4200	3609	4181.3	4180.3	3800	[J/kg K]
Thermal conductivity κ	0.58	0.561	0.52	1.1	1.1	-	[W/mK]
Blood perfusion ω	0.0005	0.0036	0.0036	0.0036	0.0036	-	[s^{-1}]
Metabolic heat Q_{met}	420	420	420	420	420	-	[W/m^3]

Table S3. Laser source parameters for the Bioheat transfer equation.

Parameters	**Values**	**Units**
Beam diameter w_o	4.5	[mm]
Laser power output	4.5	[W]
Wavelength λ	808	[nm]

Table S4. Optical properties of the tumor, the healthy tissue and skin at 808 nm*(4-7)*.

Parameters	**Skin (animal)**	**Fat (animal)**	**Thyroid Gland (human)**	**Background tissues (human)**	**Thyroid tumor (human)**	**Calculated MWCNTs within the tumor site**	**Units**
Abso. Coeff.	19	6.5	3	3	3	64	[1/m]
Scatt. Coeff.	834	1000	800	800	800	182	[1/m]
Anisotropy	0.775	0.775	0.9	0.9	0.9	-	-

References

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